Numerical Simulation of Li Diffusion in 3D Polycrystalline $LiCoO_2$

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$LiCoO_2$ is a commonly used cathode material of Li-ion rechargeable batteries. In battery applications, crystal anisotropy and grain boundaries have large influence on ion diffusion properties. To improve the battery performance, a thorough understanding of the diffusion process of Li ions is significant. In this study, 3D microstructures of various grain sizes were generated using phase field models. The apparent Li diffusion coefficient was obtained using finite element method. The relationship between the apparent Li diffusion coefficient, the grain boundary diffusivity, spatial distribution of grain orientations, and the grain size was discussed.